Entanglement in nuclear quadrupole resonance

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Abstract

Entangled quantum states are an important element of quantum information techniques. We determine the requirements for states of quadrupolar nuclei with spins >1/2 to be entangled. It was shown that entanglement is achieved at low temperature by applying a magnetic field to a quadrupolar nuclei possess quadrupole moments, which interacts with the electricfield gradient produced by the charge distribution in their surroundings.

I. INTRODUCTION

Quantum entanglement [1–3] , the most characteristic feature of quantum mechanics, is one of the central concepts in quantum information theory and is the feature that distinguishes it most significantly from the classical theory. Entanglement is now viewed as a physical resource, which provides a means to perform quantum computation and quantum communication [5] . It should be emphasized that property of entanglement can be considered regardless of the nature of qubits[6, 7].

One of the most intensively investigated systems is clusters of coupling nuclear spins [1–3] which received considerable attention as a platform for the practical implementation of a quantum computer (QC) by using nuclear magnetic resonance (NMR) technique [14–17]. The strength of the coupling (such as dipole-dipole, scalar or exchange interactions) between different spins and interaction of the spins with environment determine the decoherence time. Short decoherence times limit possible calculation times of the QC [18]. Later it has been proposed to used quadrupole nuclei, thus eliminating the requirement of interaction between spins and decreasing interaction of qubits with environment [19–25]

It was shown that a spin $\frac{3}{2}$ system is equivalent to a system of two magnetization vectors [26, 27] and can be represented using the Pauli spin matrices 2x2 [28]. It means that a single spin 3/2 is isomorphic to a system consists of two dipolar coupling spins 1/2, which can be considered as qubits. This was experimentally confirmed by using NQR technique with quadrupole splitting [21, 22]. The feasibility of quantum computing based on a pure (without external magnetic fields) NQR technique was theoretically investigated in detail in [23]. Using the resonance excitation technique and the level-crossing method, it was proposed three quantum logic gates: a controlled NOT, $SWAP$ and NOT_2 . Thus the method to synthesize qubits from a set of the spin states of a single particle with spin higher 1/2 has been developed. It is logical to raise the question of entanglement of these qubits.

Our present purpose is to investigate entanglement between the quantum states of quadrupole nuclei. We consider a nucleus with spin $\frac{3}{2}$ being in an internal electric field gradient (EFG) and an external magnetic field when the quadrupole interaction energy is of the order of the magnitude or even greater than the Zeeman one. Results of computer simulations of entanglement dynamics are presented for real spin systems with a non-equadistant energy spectrum.

II. NQR IN MAGNETIC FIELD

Let us consider a quadrupole nucleus with spin I $(I > 1/2)$ in the thermodynamic equilibrium with the density matrix

$$\rho = \mathbb{Z}^{-1} \exp\left(-\frac{\mathcal{H}}{k_B T}\right). \tag{1}$$

Here k_B is the Boltzmann constant, T is the lattice temperature, $\mathbb{Z} = Tr\left\{\exp\left(-\frac{\mathcal{H}}{k_B T}\right)\right\}$ is the partition function. In the general case, the Hamiltonian $\mathcal{H}$ can consist of the Zeeman $(\mathcal{H}_M)$ and the quadrupole $(\mathcal{H}_Q)$ parts,

$$\mathcal{H} = \mathcal{H}_M + \mathcal{H}_Q. \tag{2}$$

The Zeeman interaction between the applied magnetic field, $\vec{H}_0$ and nuclear spin is the external factor for a crystal and the direction of this field is chosen as the z-axis of the laboratory frame, $\vec{H}_0 = H_0 \vec{z}$, where H_0 is the strength of the external magnetic field. The part of the Hamiltonian describing this interaction is

$$\mathcal{H}_M = -\gamma H_0 I_z, \tag{3}$$

where γ is the gyromagnetic ratio of the nucleus with spin I, I_z is the projection of the individual spin angular momentum operators $\vec{I}$ on the z- axis.

Quadrupole coupling exists between a non-spherical nuclear charge distribution and an electric field gradient (EFG) generated by the charge distribution in their surroundings. It is possible to reduce the EFG symmetric tensor to a diagonal form by finding the principal axes frame (PAF) with the Z- and X-axises directed along the maximum and minimum of EFG, respectively, $|V_{ZZ}| \geq |V_{YY}| \geq |V_{XX}|$, where $V_{\xi\xi} = \frac{\partial^2 V}{\partial \xi^2}$ $(\xi = X, Y, Z)$ and V is the potential of the electric field. In the laboratory frame the quadrupolar Hamiltonian can be presented in the following form

$$H_Q = \frac{eQq_{ZZ}}{4I(2I-1)} U(\theta\ ,\varphi) \left[3I_z^2 - \vec{I}^2 + \frac{\eta}{2}\left(I_+^2 - I_-^2\right)\right] U^+(\theta\ ,\varphi), \tag{4}$$

where

$$U(\theta\ ,\varphi) = e^{-i\varphi Iz} e^{-i\theta Iy} e^{i\varphi Iz}, \tag{5}$$

eQq_{ZZ} is the quadrupole coupling constant of EFG, $I_\pm$ are the raising and lowering operators of the spin, and θ and φ refer to the polar and azimuthal angles determining the orientation

of the laboratory frame z-axis in the PAF coordinate system. The asymmetry parameter η is defined as

$$\eta = \frac{V_{YY} - V_{XX}}{V_{ZZ}}, \tag{6}$$

which may vary between 0 and 1.

Using the Hamiltonian (2) the density matrix (1) can be represented as a function of parameters $\alpha = \frac{\gamma H_0}{k_B T}$ and $\beta = \frac{eQq_{ZZ}}{4I(2I-1)k_B T}$:

$$\rho = \mathbb{Z}^{-1} \exp\left\{-\alpha I_z - \beta U(\theta\ ,\varphi)\left[3I_z^2 - \vec{I}^2 + \frac{\eta}{2}\left(I_+^2 - I_-^2\right)\right]U^+(\theta\ ,\varphi)\right\}. \tag{7}$$

The density matrix (7) can be employed to obtain information on the dependence of entanglement on the magnetic field, quadrupole coupling constant, orientation of the crystal principal axis in the laboratory frame, and temperature.

Below we consider entanglement in a system of spins 3/2. A suitable system for studying by NQR technique is a high temperature superconductor $YBa_2Cu_3O_{7-\delta}$ containing the ^{63}Cu and ^{65}Cu nuclei with spin $\frac{3}{2}$ possessing quadrupole moments $Q = -0.211 \times 10^{-24}$ cm^2 and -0.195×10^{-24} cm^2, respectively [32]. There are two different locations of copper ions in this structure: the first are the copper ion sites at the center of an oxygen rhombus-like plane while the second one is five-coordinated by an apically elongated rhombic pyramid. The four-coordinated copper ion site, EFG is highly asymmetric ($\eta \geq 0.92$) while the five-coordinated copper ion site, EFG is nearly axially symmetric ($\eta = 0.14$). The quadrupole coupling constant (eQq_{ZZ}) of ^{63}Cu in the four-coordinated copper ion site is 38.2 MHz and in the five-coordinated copper ion site is 62.8 MHz [32].

III. REDUCED DENSITY MATRIX AND MEASURES OF ENTANGLEMENT

An important measure of entanglement is the concurrence [33]. The concurrence C is usually used [33]. For the maximally entangled states, the concurrence is $C = 1$, while for the separable states $C = 0$. The concurrence of a quantum system with the density matrix presented in the Hilbert space as a matrix 4×4 is expressed by the formula [33]:

$$C = \max\left\{0, 2\nu - \sum_{i=1}^{4} \nu_i\right\} \tag{8}$$

where $\nu = \max\{\nu_1, \nu_2, \nu_3, \nu_4\}$ and ν_i $(i = 1, 2, 3, 4)$ are the square roots of the eigenvalues of the product

$$R = \rho_{red}\tilde{\rho}_{red}, \tag{9}$$

where $\rho_{red} = Tr_{partial}(\rho)$ is the reduced density matrix, $Tr_{partial}(...)$ is the partial trace, and

$$\tilde{\rho}_{red} = G\bar{\rho}_{red}G \tag{10}$$

where $\bar{\rho}_{red}(\alpha, \beta)$ is the complex conjugation of the reduced density matrix ρ_{red} and

$$G = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}. \tag{11}$$

An another important measure of entanglement is the entanglement entropy. In order to implement this measure of entanglement we first map the Hilbert space of a spin 3/2 which is four dimensional onto the Hilbert space of two spins 1/2, S_A and S_B [36]. The entropy of entanglement is defined as [34, 35]:

$$E = -Tr\left(\rho_A \log_2 \rho_A\right) = -Tr\left(\rho_B \log_2 \rho_B\right). \tag{12}$$

Here ρ_A is the partial trace of $\rho_A = Tr_B(\rho)$ over subsystem B, and ρ_B has a similar meaning.

This entropy is related to the concurrence C by the following equation [33]

$$E(x) = -x\log_2 x - (1-x)\log_2(1-x), \tag{13}$$

where $x = \frac{1}{2}\left(1 + \sqrt{1 + C^2}\right)$.

The numerical simulations of entanglement of the spin states are performed for special case $I = 3/2$ using the software based on the *Mathematica* package. In the equilibrium the states of the system determined by Eq. (7) are separable without applying external magnetic filed $(\alpha = 0)$ at any temperature. At large temperature $(\beta < 1)$ and low magnetic field strength $(\alpha < 1)$ the concurrence is zero. Entanglement appears in the course of temperature decrease and increasing the magnetic field.

The concurrence and the entanglement of formation dependences on the magnetic field, quadrupole coupling constant, and temperature is qualitatively independent of the angles. As example, we present below the concurrence as a function of the parameters α and β

for the concurrence maximum for a spin in the five-coordinated copper ion site ($\eta = 0.14$) at $\theta = 0.94$ and $\varphi = 0$ (Fig. 1). The concurrence and the entanglement of formation increase with the magnetic field strength and inverse temperature and reache their maximum value. Then the concurrence and the entanglement of formation decrease with increasing the magnetic field strength (Fig. 2). Another dependence of the concurrence and the entanglement of formation on temperature is observed (Fig. 3). At a high temperature concurrence and the entanglement of formation are zero. With a decrease of temperature below a critical value the concurrence and the entanglement of formation monotonically increase till a limiting value. The critical temperature and limiting value are determined by a ratio of the Zeeman and quadrupole coupling energies, α/β.

IV. DISCUSSION AND CONCLUSIONS

The obtained results show that the entangled states can be generated between the states of a single nuclear spin $\frac{3}{2}$. From a point of of view of quantum information processing the considered system is isomorphic to a system consisting of two dipolar coupling spins $\frac{1}{2}$. The same quantum logical gates can be realized using the both systems. Therefore the obtained entanglement can be considered as entanglement between qubits formed by states of a single particle. On the other hand, a single spin 3/2 isomorphic to a system consists of two dipolar coupling spins 1/2 and entanglement between the states of a spin 3/2 can be considered as entanglement between two effective spins 1/2. The behavior of entanglement of a spin 3/2 is very similar to that for the system consisting of two dipolar coupling spins $\frac{1}{2}$ [37]. It was obtained that in zero magnetic field the states of the both spin systems, two spins $\frac{1}{2}$ and spin $\frac{3}{2}$, are in separable states. These systems become entangled with increasing the magnetic field. Then, with a further increase of the magnetic field the spin states of the both systems tend to a separable one.

It has recently been shown that, in a system of nuclear spins $s = 1/2$, which is described by the idealized XY model and dipolar coupling spin system under the thermodynamic equilibrium conditions, entanglement appears at very low temperatures $T \approx 0.5 \div 0.3$ μK [37, 38]. In a non-equilibrium state of the spin system, realized by pulse radiofrequency irradiations, estimation of the critical temperature at which entanglement appears in a system of spins $\frac{1}{2}$ gives $T \leq 0.027$ K [39]. The calculation for ^{63}Cu in the five-coordinated

copper ion site of $YBa_2Cu_3O_{7-\delta}$ at $\alpha/\beta = 1$, $\eta = 0.14$ and $eQq_{zz} = 62.8$ MHz, gives that the concurrence appears at $\beta = 0.6$ (Fig. 4). This β value corresponds to temperature $T \approx 5$ mK. This estimated value of critical temperature is by three orders greater than the critical temperature estimated for the two dipolar coupling spins under the thermodynamic equilibrium [37].

In conclusion, performing investigation has shown that entanglement can be achieved by applying a magnetic field to a single spin 3/2 at low temperature. Concurrence and the entanglement of formation depend on the orientation between the external magnetic field and PAF axes. At $\theta = 0$ and π the states are separable at any conditions. At $\eta = 0.14$ the concurrence and the entanglement of formation reache their maximum value at $\theta = 0.94$ and $\varphi = 0$ and π . This effect can open a way to manipulate with the spin states by a rotation of the magnetic field or a sample.

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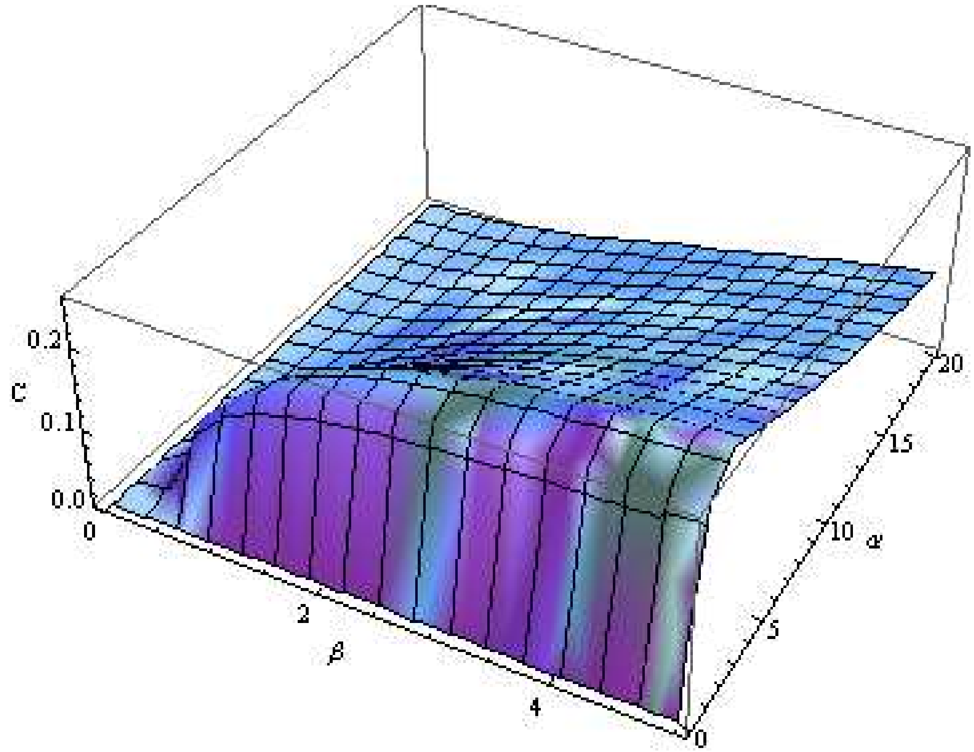
Figure Captions

Fig. 1 (Color online) The maximum concurrence as a function of the parameters α and β at $\eta = 0.14$, $\theta = 0.94$, $\varphi = 0$.

Fig. 2 (Color online) Concurrence (a) and the entanglement of formation (b) vs. magnetic field at $T =$ const for various quadrupole interaction constants: black solid line – $\beta = 2$; red dashed line –$\beta = 6$; green dotted line – $\beta = 8$; blue dash-doted line – $\beta = 12$.

Fig. 3 Concurrence (a) and the entanglement of formation (b) as a function of temperature at $\frac{\alpha}{\beta} = 0.5$ (black solid line), $\frac{\alpha}{\beta} = 1$ (red dashed line), and $\frac{\alpha}{\beta} = 2$ (blue dotted line) at $\eta = 0.14$, $\theta = 0.94$, $\varphi = 0$ Temperature is given in units of $\frac{eQq_{ZZ}}{4I(2I-1)k_B}$.



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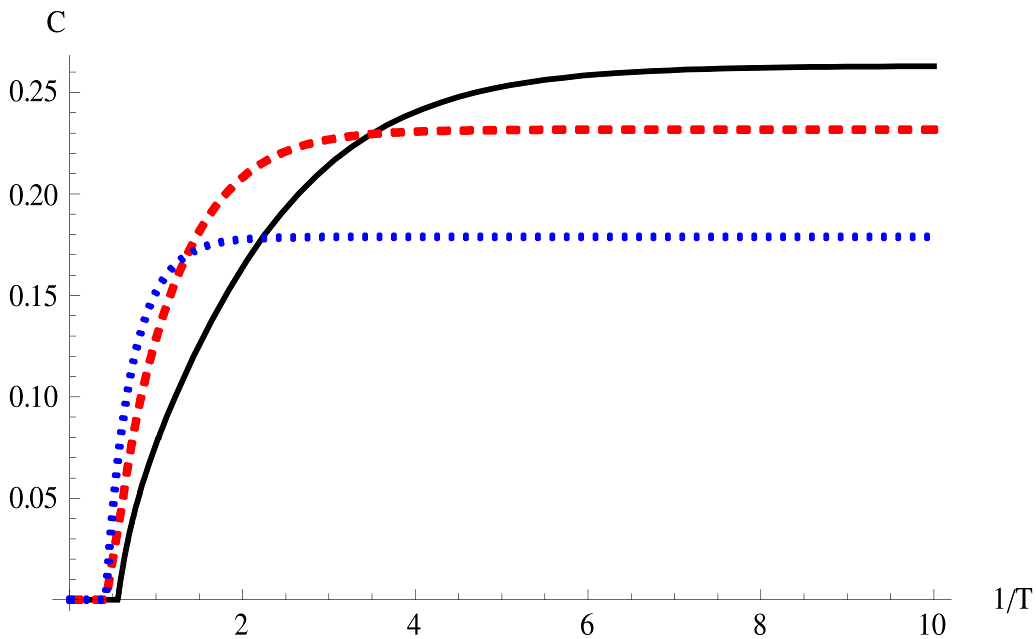
(a)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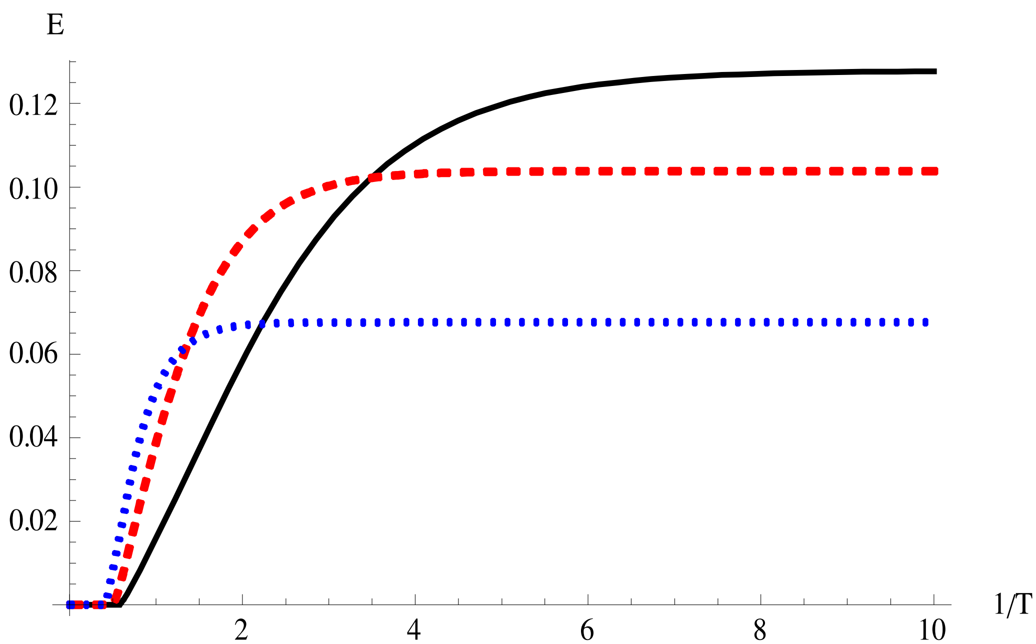
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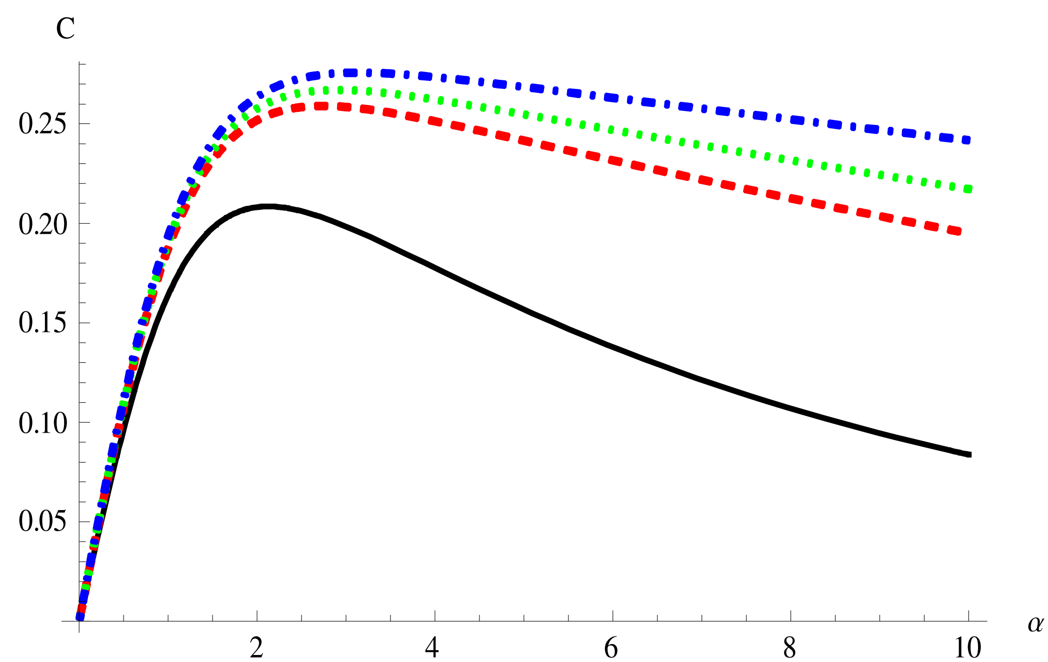
(a)



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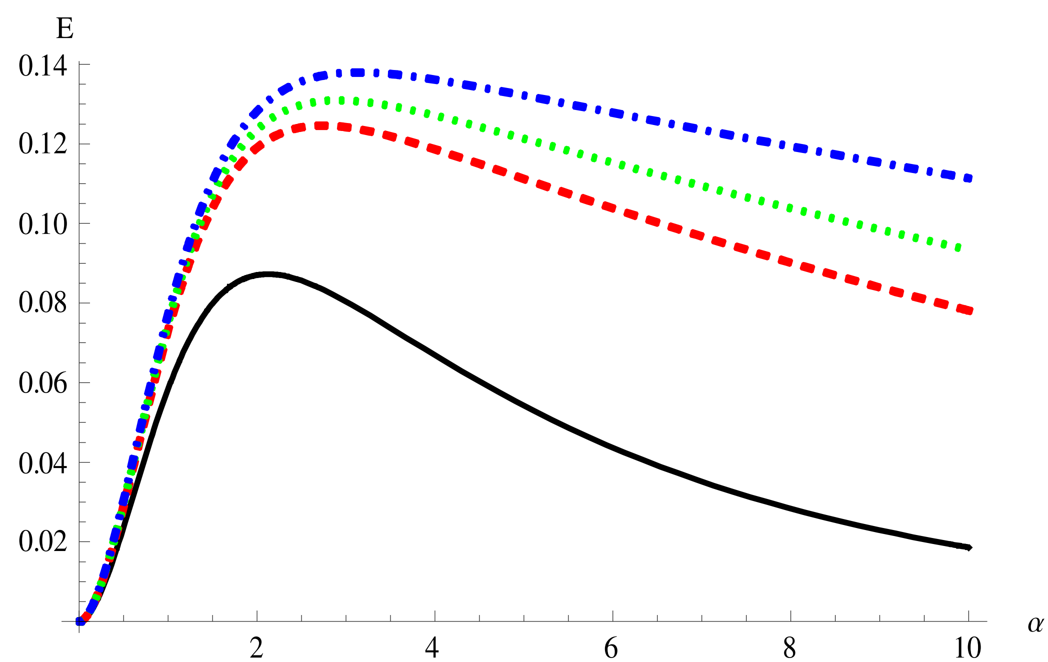

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